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AASERT95/DOCTORAL RESEARCH IN WAVELET NDE AND NOVEL DIELECTRICS

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13. ABSTRACT (Maximum 200 words)

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The goals of this project were to perform and publish mathematical research on wavelet signal processing, periodic composite dielectrics, and complete some work on the dispersion of water form a previous AFOSR grant. The wavelet studies were directed toward non-destructive evaluation using ultrasonic waves. The novel dielectrics were mainly the PBGS, photonic band structures-periodic arrays of a dielectric with permittivity e_a embedded in a background dielectric with permittivity e_b. Several types of disorder of these periodic objects were also studied.

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March 30,1999

Dr. Jon Sjögren

AFOSR/NM

801 Randolph St., Room 732

Arlington, VA 22203-1977

Dear Dr. Sjögren:

Bernadette, Please log & accept this final report with copies to DTIC. I put one copy already in case folder. JS

Enclosed please find the final report for Research grant #AFOSR/NM 49620-95-0380. Thank you for providing the research support, which was much appreciated. I specially appreciated working with a supervisor who understood the work we are doing .

With best regards,

Brian DeFacio

Brian DeFacio

Professor and PI

FINAL REPORT SF 298
AFOSR/NM Grant F49620-95-0380

Doctoral Research in Wavelet NDE

and Novel Dielectrics

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1. OBJECTIVES:

The goals of this project were to perform and publish mathematical research on wavelet signal processing, periodic composite dielectrics, and complete some work on the dispersion of water from a previous AFOSR grant. The wavelet studies were directed toward non-destructive evaluation using ultrasonic waves. The novel dielectrics were mainly the PBGS, photonic band structures - periodic arrays of a dielectric with permittivity e_a embedded in a background dielectric with permittivity e_b. Several types of disorder of these periodic objects were also studied.

2. STATUS OF THE EFFORT:

There are eleven publications, two submitted manuscripts and two more in preparation for this project. There have been a number of invited talks presented, including one at Oberwolfach, Germany; a Gordon Conference in New England; three 90-minute lectures in Madeira and two 50-minute talks at special sessions of the American Math Society at Iowa City and Albuquerque as well as three talks at the annual QNDE meeting. A number of other talks, colloquia and seminars have also been presented on the work done on this grant.

Two students who have worked on this project have graduated. Dr. Alan Van Nevel graduated in August 1996 and Dr. Sankar Chakraborty graduated in June 1997. Dr. Van Nevel, who was supported by this AASERTS grant, received an American Society for Engineering Education Fellowship at the Naval Weapons Laboratory in China Lake, CA upon graduating, and is now a permanent member of their scientific staff. Dr. Chakraborty joined a Positron Emission Tomography group at Washington University in St. Louis as a postdoctoral fellow in medical physics. He is now a postdoctoral fellow in the Radiology Dept. of the Harvard University Medical School. These two PhD's are a worthy accomplishment on this grant. A postdoctoral fellow at Missouri, Dr. Sarah John, who was also supported by this grant, has come into her own during these three years. Her research was a big project, as will be shown later in this report.

3. ACCOMPLISHMENTS:

The work on this grant has produced several discoveries. The numbers [A], {A = 1,2,...,15} denote the publications, submitted manuscripts, and manuscripts in progress listed in the PUBLICATIONS section of this report. The work on this proposal was enhanced by a research leave from Missouri University to spend the academic year 1997-98 at the Mathematics Department of Texas A&M University. This competitive leave provided 2 semesters of research at full salary. Conversations and consultation with Professors Battle, Dobson, Narcowich, Larson and others were both informative and enjoyable. The first task of this project was to read and correct the proofs of papers [1-3]. Chakraborty and I then worked on the idea for the generalization of the statistical mechanics of the permitivity of water to aqueous biomolecular solutions [6], which was worked out and published.

The most interesting discovery was a <u>dielectric hysterisis</u> effect in aqueous solutions of hemoglobin in the microwave frequency range. The simpler biomolecules Glycine and Myo-globin solutions do not show any signs of this effect.

During this time, H. Kaiser's research group at the Missouri University reactor had some interesting questions about neutron optics which led to paper [4] and later to paper [8]. In [8] a full wavelet analysis of the neutron-scattering data of a layered metallic composite was published. In another area, reference [9] has developed into one of my best papers. It extends and generalizes a number of results on the so-called "Feynman path integral" for the time evolution

$$x(t) = [\exp(-tA)](x(0)) \tag{1}$$

of a solution x where A is on an anti-self-adjoint infinitesimal generator of time translations. The operator A is the sum of two or more non-commuting, possibly time-dependent operators. Some results were obtained for non-linear and for spatially non-local parts of A. Theorems were

given which prove the existence and uniqueness to a broader class of these evolution solutions than was previously known. Explicit formulae were given for a number of realistic cases, which do not seem to have been known. A number of combinorical formulas were derived in this work using the generalized Baker-Campbell-Hausdorff equations which we found and proved.

In Van Nevel's dissertation studies [5,7,12] and in our recent continuations, [8], the behaviour of the wavelet scale variable was investigated for ultrasonic backscatter for nondestructive evaluation. The scale is the "new" structure of wavelets which Fourier signal processing lacks. The change from one scale to another corresponds to zooming in and out. The initial idea was that the features one seeks in the data are zeros, maxima and minima. Thus, small coefficients are required in some scales to accurately determine these features. One would expect high frequency scales for fine details, so the following empirical procedure was tested with hundreds of time traces provided by Prof. Neal of the Dept. of Mechanical and Aerospace Engineering here. The scales present in these ultrasound scans were **0-8** (256 data per scan), or **0-9** (512 data per scan) for $p = 2$ wavelets where $j = 0$ to 8 or $0 = 9$ in the scale 2. The scales which were left unchanged were called exceptional scales and the rest were called ordinary scales. A threshold, **e** which depended only on the on the signal-to-noise ratio was easily found. The best choice of exceptional scales were found to be $j = 3,4,5$. This was unexpected, so it was checked again and again. The additional study served to confirm this choice. Another study was undertaken to see if there was a "best" wavelet without success. It was found that **CN, DSN, DN** wavelet s with a lot of smoothness tended to perform better; ie. **N>>1 (10-28)**. This was interesting, and probably will prove useful, but is not a satisfactory physical theory. Why these scales and not others? The Shannon information was studied but failed to improve simple suboptimal Wiener filtered reconstructions of backscattered amplitudes. Some estimates by Donoho and co-workers fared even worse. This experience pointed us in the right direction. The Shannon information proved to be largely redundant with the energy error norm: it added no new information. This would explain why the Shannon information added so little to these inversions. The Donoho approach used some of the understanding on ultrasonic scattering which has been built up in the past 20-25 years. This gave us the idea to try the Kullback-Liebler information I_{KL}. Let **P** be a probability distribution made from Wiener filter reconstructed scattering amplitudes , where p_i **P** is the real or imaginary part of the backscattered signal. Let **Q** be a reference probability distribution q_i **Q** where q_i is a real or imaginary part of a suitably normalized calculated

ultrasound backscattered signal. The Kullback-Liebler information in bits is given by

$$I = - \Sigma_i p_i \log [p_i/q_i] \tag{2}$$

Dr. Van Nevel expanded p_i's and q_i's in wavelet coefficients and maximized I_{KL} wavelet scales j and translations k. This turned out to leave most of the small coefficients in the scales $j=3,4,5$ and improved the Wiener filter markedly. For example, the (real, imaginary) l^2 error norm were decreased from (0.8692, 1.2415) to (0.1723, 0.2513) for the C18 wavelet family. The values of j and k with large and/or exceptional wavelet scales form an information ; energy island in the wavelet phase space. This method removed much of the noise from the reconstructions.

Several other methods were studied. Both a Monte Carlo method and a simulated annealing method were found by Van Nevel to perform comparably to the empirical scale choice and the Kullback-Liebler information maximization. They are non-trivial, but require much more expertise and computer time to apply. Although it is reassuring to see that all of these methods leave many of the small coefficients in scales in $j= 3,4,5$; the only explanation which has been found so far is the Kullback-Liebler information. This justifies the intuition in the original proposal that the total inverse reconstruction minimizes the l^2 error in the scattered energy or pressure and the information jointly, subject to the constraint of keeping the energy at the level indicated by the SNR estimate. The only information required is the approximate SNR and a known threshold, e_t.

Dr. John published [11] which used dilations of a lattice to completely work out the sampling properties of compactly supported, orthonormal wavelets. The fact that lower N wavelets contain aliasing errors was known, but not to what extent. John worked this out in full detail. She proved that only the **D** satisfies the Shannon sampling rate. This Shannon wavelet is not compactly supported because it has **X-** . Dr. John also found that the correct choice; **SU(2)** group structure of the filters rules out the pathological cases which Madysch pointed out. Daubechies had known of their existence, according to Prof. Madysch. The half-angles of **SU(2)** matrices force these cases, and only these, to zero as shown in John's paper. She thus showed

that they are an artifact of the wrong group choice for the filter matrices. The aliasing argument in this paper partially explains why higher **N**-wavelets perform better in our reconstructions. Besides their finer detail from additional smoothness, they also have smaller aliasing errors.

The two more competent dielectrics, or *photonic crystals* are a new class of materials whose *light* or *optical* qualities can be designed and controlled. This basic knowledge will make new, fast devices for switches, high **Q**-tuning, filters, communication, and computation. The bandgap completely suppresses all noise whose wavevector or energy, **k** or **E**, are in the forbidden gap. This fact is physically rigorous because the noise is electromagnetic radiation emitted from atoms. Photonic crystals change the environment of the atoms, which shift their energy levels and make certain frequency regions of noise impossible because they correspond to non-existent solutions.

The Photonic Band Structure project is going full steam, thanks to the energetic work of Sankar Chakraborty [10,13,15]. Regular consultation with Prof. A. Figotin (an AFOSR/NM contractor at California-Irvine) continues being valuable to this project. A beautiful paper by Figotin on the spectral of PBGS showed the PI how limited the theoretical physicist's approach is on this subject. Figotin's theorem that two-component dielectrics with *space-filling structures at high dielectric contrast* , ie. squares in square lattices at high dielectric contrasts maximize the bandgap is a major landmark in PBGS. Unfortunately, his group and ours are the only ones using this fundamental structural feature. Part of our long-term agenda is to show engineers, device technologists, and theoretical physicists how useful these analytical results are in practice. For example, the abstract proof in scaled space-filling structure is greater than a corresponding non-space-filling case, but it cannot show how much because the model is quite complicated. If is small, **<1%**, then it is not of practical consequence. We have shown that it is **>10%** , which is quite significant. There is much more to learn on this subject, including localized defects and localization.

Chakraborty and the PI have three ways to solve the matrix discretizations of Maxwell's equations in the two periodic dielectric regions: plane wave expansions; exact solutions for small, square lattices; and variational methods using trial functions made of linear combinations of spherical or cylindrical **Mie** scattering vector spherical harmonics. The plane vector solutions are most versatile for large systems containing many periodic scatterers. The exact solutions are

complementary to plane waves, since they are only useful for small numbers of scatterers and are limited in the number of scattering shapes which can be solved exactly. The exact solutions have also been used for checking the accuracy of other approximations. The variational method is useful for the two shapes which cannot be exactly solved. They have the desirable feature that $\omega(\text{var}) > \omega(\text{exact})$ but quickly lose accuracy as one goes to higher frequencies than the first ten bands.

All possible symmetric scatterer shapes have been calculated in all 2D lattices. The **3D FCC** lattice has been solved. It is interesting that the theoretical physics literature contains only plane wave calculations at a few filling factors **f** for a few pairs of dielectrics. (e_a, e_b), mainly **GaAs, Ge, Si,** which are high-technology device materials. Most authors claim 2-3% accuracy and some show 12-15 bands, yet different authors differ by $+(15\text{-}20)\%$ from one another for the same PBGS structure! Here the internal fields **D(r)** and the density of states have been calculated and a number of new discoveries have been made. Some work on elastic waves, filters and oscillators have also been completed, while others are in progress. These have been relegated to the next section.

Since the PI has studied elastic wave propagation for over 20 years for NDE studies, we formulated the PDE's for some 2-D periodic elastic composites. These devices have forbidden band gaps (stop bands), localized defects, and, possibly, localization phenomena for elastic waves.

We seem to be the only people studying biological materials in PBGS. In the microwave frequency window these systems have strong dispersion and attenuation (dissipation) which provide new physical effects. One of these is the opening of a frequency gap in the dispersion spectrum of a **3D FCC** lattice. Another is the strong spatial dispersion in the attenuation $\alpha(\omega, \mathbf{k})$. The effects of wavevector lattice disorder in the response frequency and gap widths are greatly increased. However, the gap divided by the mid-gap frequency decreases as it must by a theorem of Figotin and Klein. Transmission effects and localized defects have also been calculated for acoustic, electromagnetic and elastic waves.

Some of the follow-on projects that directly further the mission of the Air Force include:

1. Generalized entropies and information with an understanding of the independence and redundancy of the information from the energy error norm. Study NDE to avoid "theoretical nonsense". Study real data for transient pulses.

2. Matched wavelet filters for NDE.

3. Resonant ultrasound spectroscopy inverse problem for determining the elastic stiffness constants accurately.

4. Renormalization group - wavelet analysis to tailor wavelets to problems such as PBGS, topic (2) above, and a deeper understanding of the scale variable.

4. PERSONNEL SUPPORTED:

Brian DeFacio, PI; 2 months a year for 3 years

Sarah John, Visiting Asst. Professor; half time for 3 years

Sankar Chakraborty, graduate student/PhD; 2 months a year for 3 years

Stefan Gheorghiu, graduate student; 2 months a year for 3 years

Alan Van Nevel, graduate student/PhD; this AASERTS grant for 2 years

Eric Veum, graduate student; AASERTS grant for 6 months

Elijah Flenner, graduate student; AASERTS grant for 6 months

5. PUBLICATIONS;

1. S.-H. Kim, G. Vignale and B. DeFacio, <u>Dynamic Dielectric Response of Liquid Water,</u> Phys.Rev, **E50**, 4618-4624 (1994).

2. B. DeFacio, S.-Kim, and A. Van Nevel, "Applications of Squeezed States - Bogo- liubov Transformations of the Statistical Mechanics of Water and Its Bubbles", Intnl. Wkshp. on Squeezed States & Uncertainty Rel. in *NASA Conf.Proc.*; D.Hsan, M. Rubin, Y.Shin, and M.A. Man'kov, eds. 339-351(NASA, Greenbelt MD,1994).

3. B. DeFacio,"Coherent-state Path Integrals and their Relation to Wavelets" in On Klauder's Path: A Field Trip, G.G. Emch, G.Hegerfeldt, and L. Streit, eds.,43-53 (World Sci.Pubs., NY,1994).

4. H.Kaiser, K.Hamacher, R.Kulasekere, W.-T.Lee, J.F.Ankner, B. DeFacio, P. Miceli and D.L. Worcester,"Neutron Inverse Optics in Layered Materials," in Inv. Optics III; M.Fiddy, ed., SPIE **2241**, 78-89 (Soc.Photo.Ind.Engr., Bellingham,WA,1994).

5. D.M.Patterson and B. DeFacio,"Wavelet Inversion of Data for Elastic Wave Non destructive Evaluation," in Inverse Optics III, M.Fiddy, ed., SPIE **2241**,172-184.

6. S, Chakraborty and B. DeFacio, "Dynamic Frequency-dependent Dielectric Response of Three Aqueous Biomolecular Solutions," Physica **221**, 449-437 (1995).

7. A. Van Nevel, B.DeFacio, and S.P.Neal,"An Application of Wavelet Signal Processing to Ultrasonic Nondestructive Evaluation," Rev.QNDE **15**,733-740 (1996).

8. G.Saab, B.DeFacio, H.Kaiser and D.L.Worcester,"Wavelet Inverse Neutron Scattering Study of Layered Metallic NiC-Ti Composites." Rev.QNDE **16**, 39-46 (1997).

9. B. DeFacio, G.W.Johnson and M.Lapidus, <u>Feynman's Operational Calculus and</u>

Evolution Equations, Acta Appl.Math., **47**, 155-211 (197).

10. S. Chakraborty and B.DeFacio, Periodic Composite Backing Filter for the Design of Ultrasonic Transducers, Rev.Prog.QNDE **17**, 875-887 (1998).

11. S. John, Lattice Functions, Wavelet Aliasing, and SO(3) Mappings of Orthonormal Filters, J.Math.Phys. **39**, 569-593 (1998).

12. A.Van Nevel, B.DeFacio and S.P.Neal, Information-theoretic Wavelet Noise Removal for Inverse Wave Scattering Theory, Phys.Rev.E **59**, (in press,1999).

13. S.Chakraborty and B.DeFacio, Electromagnetic Waves in 3-D, Periodic, FCC, 2 -Component Dielectric Structures Containing a Biological Material, (submitted, 1998).

14. B.DeFacio, J.A.Sjogren and E.Flenner, The Mobius Transformation and p=2 Wavelets for Noisy Relaxation Processes (in preparation).

15. S. Chakraborty and B.DeFacio, High Dielectric Contrast, Microwave frequency, 2-D Photonic Band Gap Structures with Dispersion, and, Possibly, Loss Tangents (in preparation).

6. INTERACTIONS:

A. Participation/presentations at meetings, conferences, etc.

1. Participant in the Program Review on Computational Electromagnetism, Brooks AFB, Jan '95,'96,'97.

2. Invited colloquium and seminar speaker on this work at the Physics Dept, University of Cinncinati, spring '95.

3. Presented talks on Wavelet Inverse Scattering, Coherent States, March meeting, Am.Phys.Soc., Indianapolis, 1995.

4. Invited speaker (3, 90-minute lectures on Wavelet Inverse Problems)European Common Market Summer School, Madeira, Portugal,1995

5. Presented talk, was session chair 1995 QNDE meeting in Seattle.

6. Presented 2 talks at St. Louis Meeting of the Am.Phys.Soc.,1996.

7. Invited speaker, Oberwolfach, Germany, summer 1996.

8. Invited participant, poster session, Gordon Research Center, 1996.

9. Presented talk, was session chair at 1996 Bowdoin QNDE meeting.

10. Presented 2 papers, was session chair at March meeting of the Am.Phys.Soc., in Kansas City, 1997.

11. Presented 50-minute talk at a special session of the Am.Math.Soc. on Localization and Other Multiple Scattering Phenomenae of Classical Waves, Albuquerque, NM, 1997.

12. "Radial Basis Functions for Elastic Wave Inverse Theory" at the Center for Approximation Theory,
    "PBGS", Condensed Matter Seminar,
    "I. Information Theory for Wavelet Inverse Problems",
    "II.InformationTheory for Elastic Waves" Atomic & Laser Seminars, Texas A&M, 1997.

B. Consulting and advisory activities at laboratories, other groups, etc.

1. Prof. A. Figotin, Dept. of Mathematics, University of North Carolina, Charlotte, on photonic band gap materials.

2. Dr. C.M.Fortunko, Nat. Inst. of Standards, Materials Reliability Division at Boulder; on
   *Analysis of transient pulses using wavelet error analysis at all stages,
   *Non-linear ultrasonics and plate Green's distributions using wavelets was being studied.
   *A more accurate experimental value of the wave propagation speed of sound.

   (Fortunko died of a heart attack in spring of 1998.)

3. Prof. Neal's Ultrasonic Laboratory at Missouri on inverse problems with ultrasound.

4. Dr. Frank Margatan, NSF, NDE Center at ISU, on grain noise scattering.

7·X TRANSITIONS:

1. The PI, with some excellent help from Van Nevel and Veum, spent time working out answers to questions and criticism by three referees at a journal on a series of measurements by Hollman and Fortunko. They are developing new resonant

methods for measuring the speed of sound more accurately than is possible today, and we intend to continue to contribute theoretical modeling and signal processing on this project.

2. Van Nevel has taken some ideas which he started developing in his dissertation and has extended them at China Lake, where he is now a member of the scientific staff. His result uses wavelet frames to detect and clarify texture in transient radar signals.

8. NEW DISCOVERIES:

Several new discoveries have been made. The dielectric hysterisis in aqueous solutions of hemoglobin at microwave frequencies and a better model for the permitivity of water were completed (from a previous project). The effects of dispersion and dissipation in photonic band gap structures were treated and were shown to open the pseudogap in water scatterers in the microwave frequency region. Wavelet methods were developed for nondestructive evaluation of high technology materials. The wavelet scales were shown to carry large information in small coefficients of the mid-range scales $j = 3.4.5$ for ultrasound scattering with data populating scales $j = 0,1...8$ (or 9). Then the maximization of the Kullback-Liebler information was shown a similar effect. We have thus shown that it is the Kullback-Liebler information which improves these conversions.

S. John gave a complete discussion of the aliasing of compactly supported, orthonormal wavelets. She showed that it is a SU(2) group for the $p = 2$ instead of the usual U(2) which removed all of the pathological multiresolutions. It is the half angles in the SSU(2) matrices which force the unwanted cases to vanish. Periodic arrays of Young's modulus and/or permitivity PBGS have been studied for their acoustic, electromagnetic and elastic wave frequency spectra. Lattice disorder, localized defects and transmission coefficients have been studied in these composites. A potential elastic wave filter utilizing the forbidden gaps was discovered. The University of Missouri is considering applying for a patent on this filter.

9. HONORS AND AWARDS:

Fellow of the American Physical Society

Listed in Who's Who in Science and Engineering

International Advisory Board, J. Non-destructive Testing and Evaluation, Elsevier
Publishers, Oxford University

Research Leave 1997-1998 Texas A&M University

10. FINAL BUDGET:

F49620-96-0380	Adjusted Budget (no cost extension)
Salary (grad. asst., software)	$8817.88
Staff Benefits	3,683.96
Travel (meetings, research collaborations)	1,788.67
GRE fee remission	1,132.15
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12a. DISTRIBUTION/AVAILABILITY STATEMENT

Approved for public release: distribution unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

Ph.D. level graduate students in applied mathematics were educated in an area of interest to AFOSR.

Wavelet inverse methods for non-destructive evaluation of high technology materials using transient pulses of ultrasound have been developed using the Kullback-Liebler information. This selects scales with small energy wavelet coefficients which have large information content. Wavelet aliasing by all compactly supported orthonormal wavelet families has been proven, and pathological multiresolutions were ruled out by hoosing the correct group for the filters, SU(2).

The PBGS, photonic band gap structures, have been studied for electromagnetic and elastic waves. These periodic, two-component dielectrics have been studied with non-zero loss-tangents (dissipation) dispersion, and lattice-disorder. Localized defects have been studied. An Elastic wave filter and a gap opened by the high contrast of water at microwave frequencies were discovered.

14. SUBJECT TERMS

Signal processing, wavelets, non-destructive evaluation, inverse problems, photonic band gap crystals.

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